

Phase space approach to solving the time-independent Schrödinger equation: Thinking inside the box

Asaf Shimshovitz

Weizmann Institute of Science

We propose a method for solving the time independent Schrödinger equation based on the von Neumann (vN) lattice of phase space Gaussians. By incorporating periodic boundary conditions into the vN lattice [F. Dimler et al., New J. Phys. 11, 105052 (2009)] we solve a longstanding problem of convergence of the vN method. This opens the door to tailoring quantum calculations to the underlying classical phase space structure while retaining the accuracy of the Fourier grid basis. The method has the potential to provide enormous numerical savings as the dimensionality increases. In the classical limit the method reaches the remarkable efficiency of 1 basis function per 1 eigenstate. We illustrate the method for a challenging two-dimensional potential where the Fourier grid method breaks down.